

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
 Data File : VX025462.D
 Acq On : 03 Dec 2021 05:13
 Operator : JC/MD
 Sample : M4918-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-40

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	32	rBV	94512	129710	15.85%	2.583%
2	1.368	42	46	50	rVB	8629	11540	1.41%	0.230%
3	1.752	104	109	116	rVB3	6624	10569	1.29%	0.210%
4	2.215	181	185	192	rVB	6703	10867	1.33%	0.216%
5	2.867	282	292	299	rVV2	4219	9753	1.19%	0.194%
6	2.959	299	307	321	rVV	80723	172983	21.13%	3.444%
7	3.117	324	333	346	rVB	34701	79478	9.71%	1.582%
8	3.764	428	439	451	rBV	24244	64691	7.90%	1.288%
9	4.318	520	530	542	rVB3	9571	29253	3.57%	0.582%
10	5.391	694	706	716	rBV	66864	193350	23.62%	3.850%
11	5.556	723	733	748	rVB	104627	304626	37.22%	6.065%
12	5.958	788	799	805	rBV	69485	184676	22.56%	3.677%
13	6.044	805	813	829	rVB	309102	818483	100.00%	16.297%
14	6.233	834	844	856	rVB4	10419	31237	3.82%	0.622%
15	6.763	919	931	943	rBV	171261	414256	50.61%	8.248%
16	8.427	1198	1204	1210	rBV2	20908	34093	4.17%	0.679%
17	8.500	1210	1216	1225	rVB7	3246	9239	1.13%	0.184%
18	8.653	1234	1241	1247	rBV	367144	567630	69.35%	11.302%
19	8.720	1247	1252	1261	rVB2	18974	31584	3.86%	0.629%
20	8.958	1282	1291	1300	rVB	24846	38770	4.74%	0.772%
21	9.049	1300	1306	1312	rBV	31790	46254	5.65%	0.921%
22	9.244	1332	1338	1343	rBV	6276	10067	1.23%	0.200%
23	9.458	1365	1373	1388	rVB2	47436	79583	9.72%	1.585%
24	9.945	1448	1453	1459	rBV	13643	20019	2.45%	0.399%
25	10.055	1465	1471	1477	rBV	369356	487354	59.54%	9.704%
26	10.195	1490	1494	1506	rBV	22058	35315	4.31%	0.703%
27	10.299	1506	1511	1518	rVB	50883	73775	9.01%	1.469%
28	10.640	1563	1567	1573	rVB	27917	38214	4.67%	0.761%
29	10.963	1613	1620	1625	rBV	9393	13684	1.67%	0.272%
30	11.079	1634	1639	1651	rBV	283405	378969	46.30%	7.546%
31	11.305	1669	1676	1679	rBV2	7050	10312	1.26%	0.205%
32	11.378	1684	1688	1695	rVV	10312	21526	2.63%	0.429%
33	11.451	1695	1700	1705	rVB	8632	11988	1.46%	0.239%
34	11.616	1722	1727	1735	rVB	12077	15555	1.90%	0.310%
35	11.756	1745	1750	1756	rVB	26746	34230	4.18%	0.682%
36	12.024	1788	1794	1801	rBV	367451	461678	56.41%	9.192%

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37	12.085	1801	1804	1809	rVB	12187	15300	1.87%	0.305%
38	12.244	1824	1830	1838	rBV	19220	25648	3.13%	0.511%
39	12.603	1884	1889	1894	rBV2	4505	8283	1.01%	0.165%
40	12.701	1901	1905	1913	rVB2	10900	15893	1.94%	0.316%
41	13.292	1998	2002	2007	rBV2	8018	11245	1.37%	0.224%
42	13.780	2075	2082	2089	rVB	13281	19684	2.40%	0.392%
43	14.640	2217	2223	2227	rBV	12954	16565	2.02%	0.330%
44	14.780	2241	2246	2252	rBV2	10406	14667	1.79%	0.292%
45	15.615	2378	2383	2387	rBV2	6186	9789	1.20%	0.195%

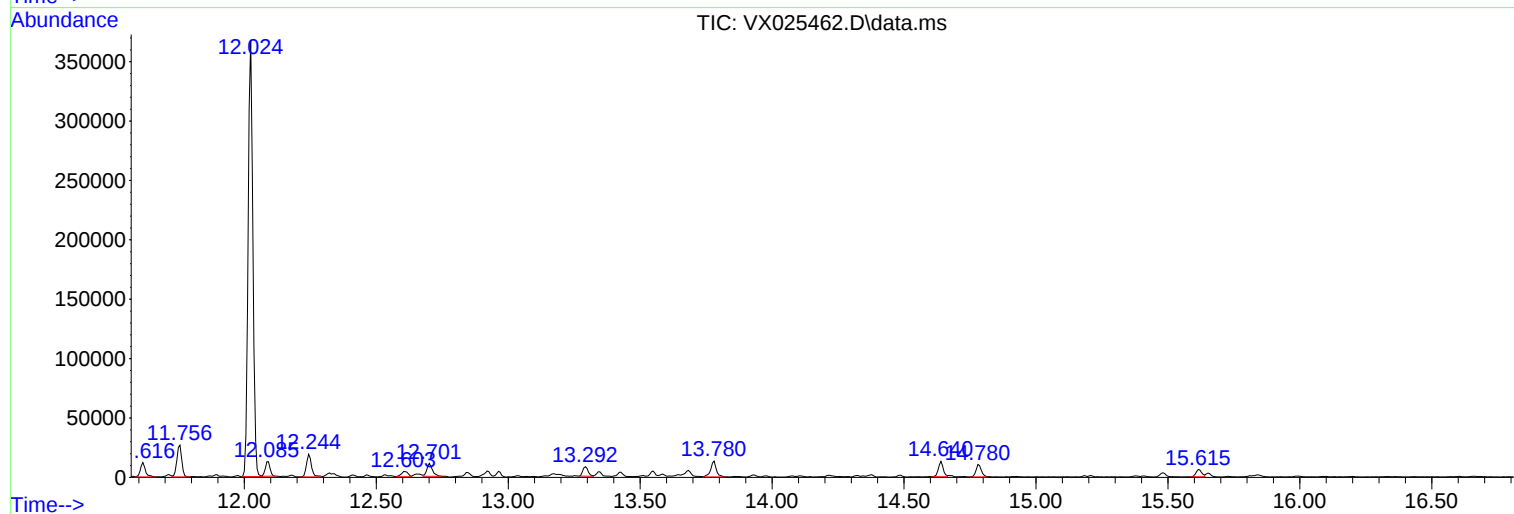
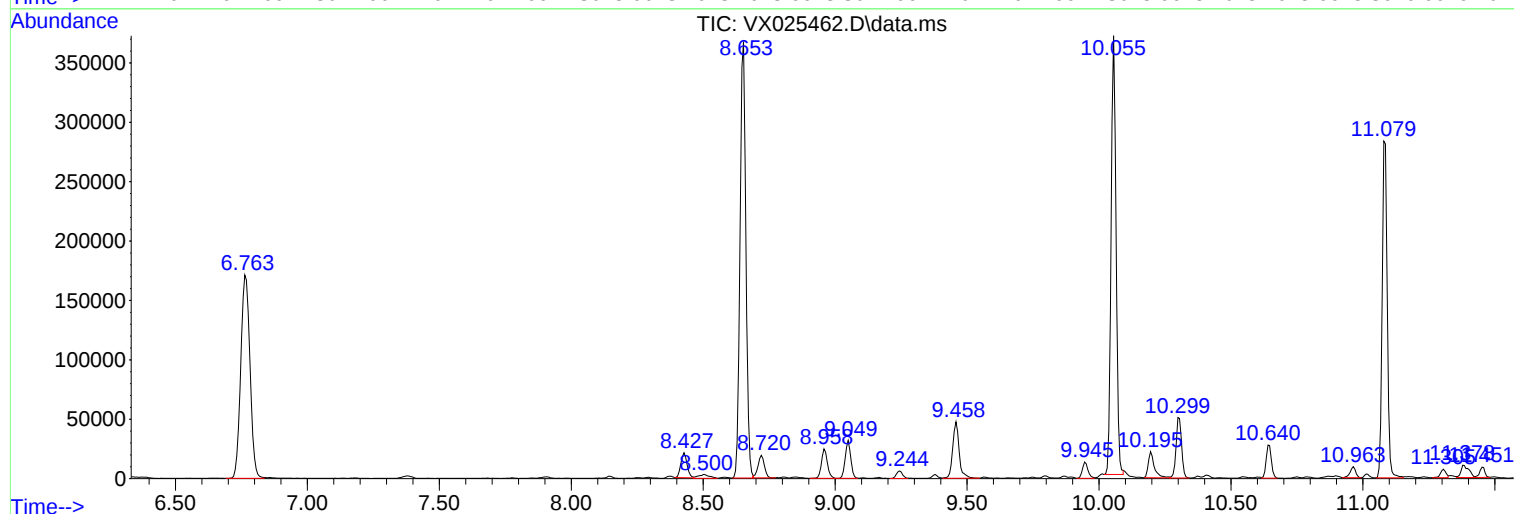
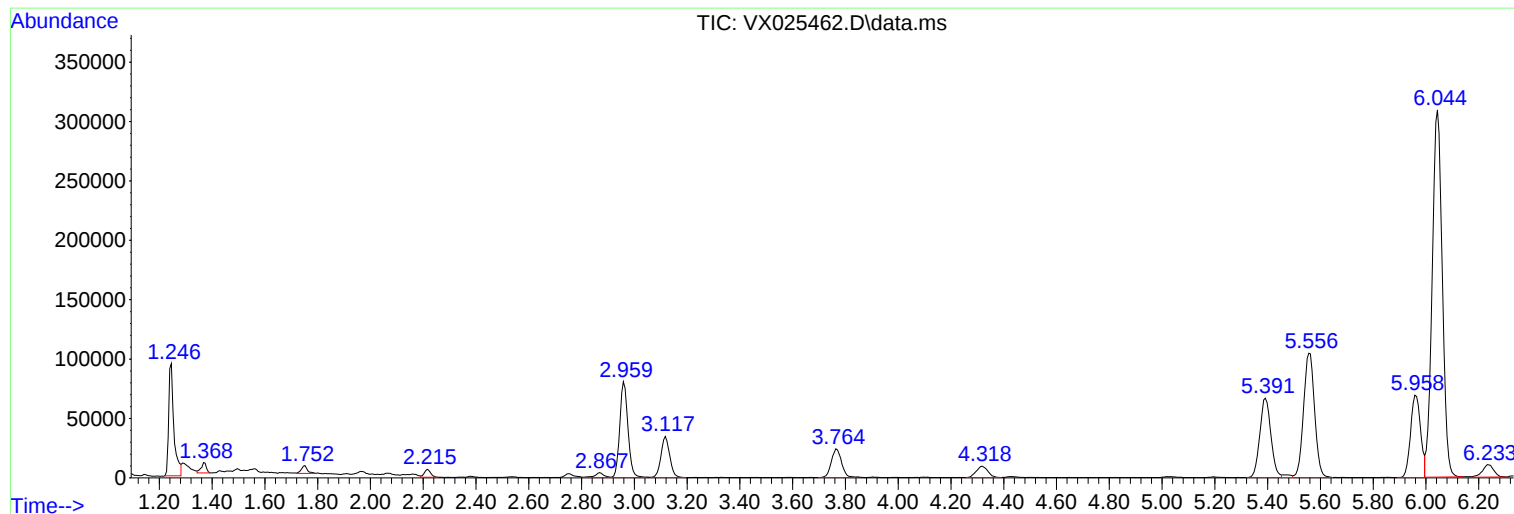
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
MW-40

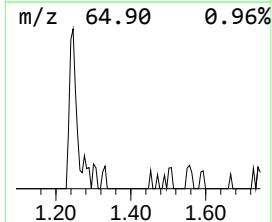
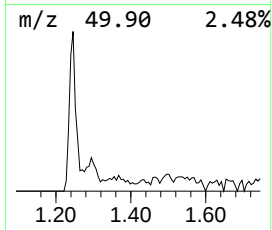
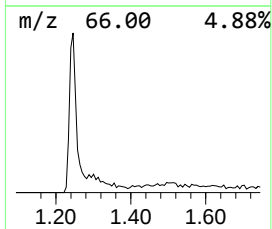
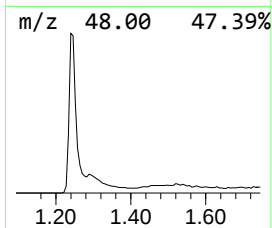
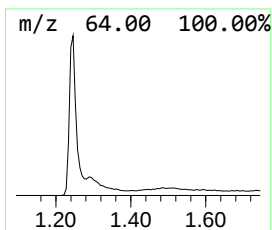
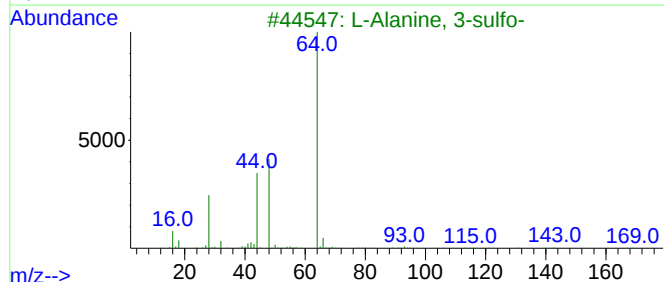
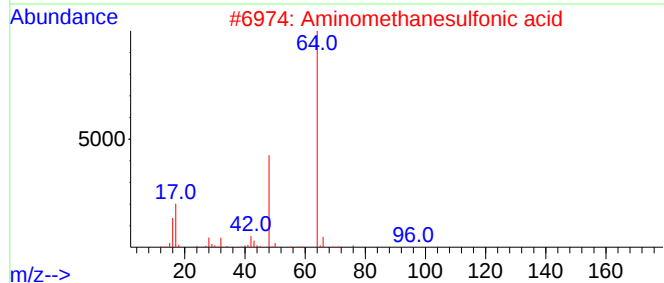
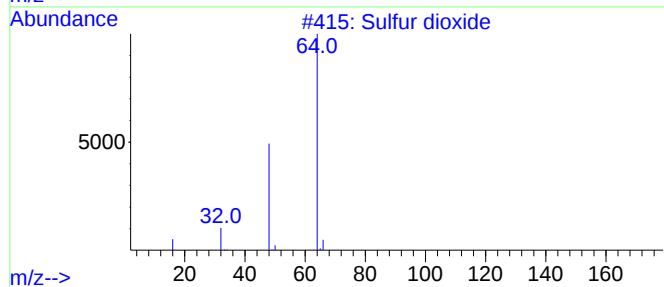
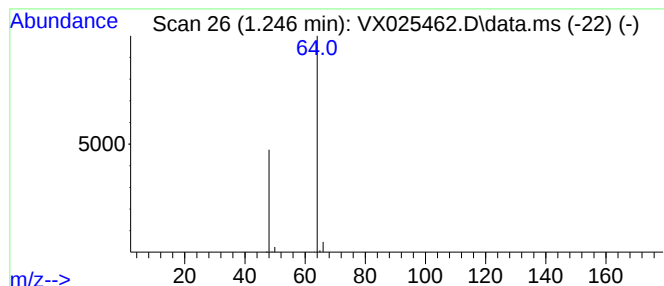
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	21.29 ug/l	129710	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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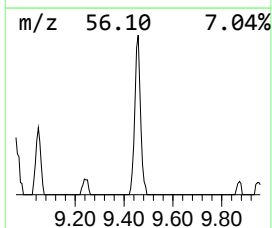
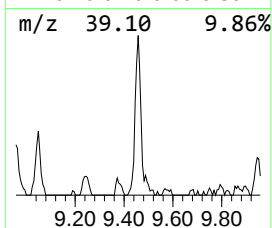
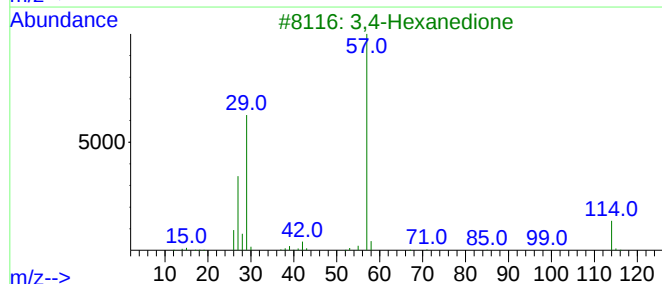
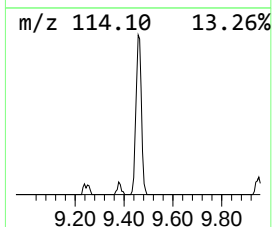
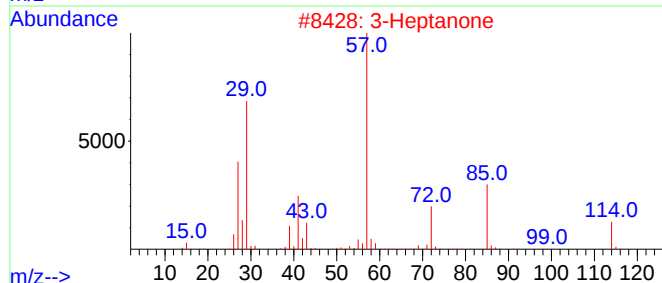
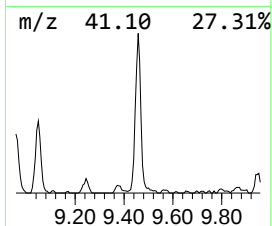
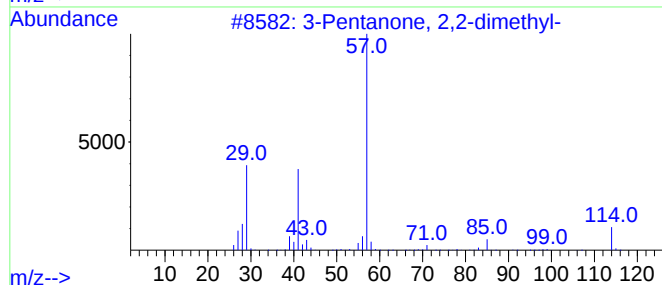
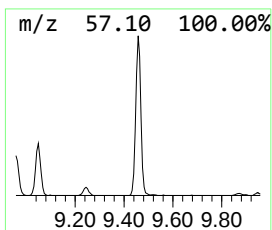
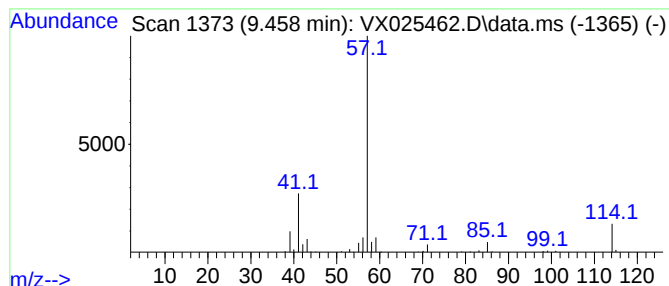
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Pentanone, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	8.16 ug/l	79583	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	83
2			3-Heptanone	114	C7H14O	000106-35-4	59
3			3,4-Hexanedione	114	C6H10O2	004437-51-8	58
4			3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	50
5			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	50



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	21.3	ug/l	129710	1	5.562	304626	50.0
3-Pentanone, 2,...	9.458	8.2	ug/l	79583	3	10.055	487354	50.0